

FRACTIONAL FACTORIAL DESIGNS

by

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Abstract

A generalized treatment of fractional factorial designs is presented. Precise definitions are given, and within this framework the subject of fractional replication of factorials is formulated. Construction and optimality properties of fractional replicates are discussed in some detail.

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Introduction

Ever since Fisher [1926] introduced the notion of "factorial experimentation" a tremendous development of ideas in this area has taken place. In factorial experimentation (originally called "complex experimentation" by Fisher), several factors may be studied simultaneously instead of experimenting with them one at a time. For example, in an agricultural experiment we may assess the effects of nitrogen and phosphate fertilizers on the yield of wheat by carrying out an experiment with various combinations of levels of the two fertilizers. If the experimenter specified k_1 levels of the nitrogen fertilizer and k_2 levels of the phosphate fertilizer and all the $k_1 \cdot k_2$ combinations are used in the experiment, then such an experiment is called a "complete factorial". If fewer than the $k_1 \cdot k_2$ combinations are used, then the term "fractional factorial" has been used in the literature for such an experiment.

Yates [1935] provided the first comprehensive approach to complete factorials and also presented some ideas in fractional factorials. It was Fisher [1942], however, who systematically constructed classes of fractional factorials, where each of the factors had the same prime number of levels. These designs came about as a by-product of the construction of "confounded designs". The formal approach to fractional factorial designs is due to Finney [1945]. Since then numerous authors have made contributions in

resolving some of the ensuing problems.

Many problems in factorial theory turn out to have a geometric, algebraic or combinatorial flavor. As a consequence mathematical structures, such as finite groups, finite rings, finite fields and finite geometries, can be successfully used in elucidating and resolving many issues. Fisher [1942, 1945] used finite Abelian groups and Bose [1947] relied heavily on finite Euclidean and finite projective geometries in the construction and enumeration of "regular fractions" of symmetrical prime powered factorials. More recently, a general algebraic-combinatorial theory of fractional factorials has been developed by Pesotan, Raktoe and Federer [1975]. This theory relied on some invariance results of Srivastava, Raktoe and Pesotan [1976] and several unsolved problems associated with it have been reported by Raktoe and Pesotan [1974].

In the sections below a systematic discussion is presented on the most important aspects of fractional factorials.

Factorial Arrangements and Fractional Factorial Designs

In this section use is made of the notation and definitions which were developed by Raktoe, Hedayat and Federer [1973] in an unpublished monograph. Since then, these authors have used it in two papers, namely, Hedayat, Raktoe and Federer [1974] and Federer, Hedayat and Raktoe [1975].

A distinction will be made between sets and collections. In a set there is a listing of distinct elements, while in a collection repetitions are allowed. In many scientific investigations experimenters are interested in studying the effects of t controllable variables. Such variables will be called factors and they will be denoted by F_1, F_2, \dots, F_t . For each factor there will be a specified range of values of interest to the experimenter. These sets of values will be called levels of the factors and they will be

indicated by G_1, G_2, \dots, G_t . A factor will be called quantitative if the underlying levels of interest are real numbers and qualitative if the levels are specified qualities rather than real numbers. Denote the cardinality of G_i by k_i , and throughout the development assume that the G_i 's are finite sets. The sets of levels G_1, G_2, \dots, G_t are potential levels and it is not necessarily true that all of them will be used in a particular experiment.

Let G be the Cartesian product of the G_i 's, i.e., $G = \prod_{i=1}^t X_i$, where the symbol X denotes the Cartesian product. The set G together with the F_i 's is often referred to as the $k_1 \times k_2 \times \dots \times k_t$ factorial or $k_1 \times k_2 \times \dots \times k_t$ crossed classification. An element of G is called a treatment and G itself is called the factor space or space of treatments. In the literature, the terms "treatment combinations", "assemblies", "runs" and subclasses" are also frequently used for treatments.

Let N be the cardinality of G , i.e., $N = \prod_{i=1}^t k_i$, and let G be indexed by the index set $\{1, 2, \dots, N\}$. Then a factorial arrangement or factorial design with parameters $k_1, k_2, \dots, k_t, m, n, r_1, r_2, \dots, r_N$ is defined to be a collection of n treatments such that the j th treatment of G has multiplicity $r_j \geq 0$, m is the number of non-zero r_j 's, and $\sum_{j=1}^N r_j = n > 0$. A factorial arrangement is denoted by the symbol $FA(k_1, k_2, \dots, k_t; m; n; r_1, r_2, \dots, r_N)$ or simply by FA if everything is clear from the context.

In the discipline of statistics the multiplicity r_j is referred to as the replication number of the j th treatment, i.e., how many times the j th treatment is repeated in the factorial arrangement. The definition of a factorial arrangement adopted here is in complete agreement with the definition of a general t -way crossed classification with r_j observations on the j th treatment.

A factorial arrangement is said to be a complete factorial arrangement

or a complete replicate if $r_j > 0$ for all $j = 1, 2, \dots, N$. It is said to be a minimal complete factorial arrangement if $r_j = 1$ for all j . Note that a minimal complete factorial arrangement is a single copy of the factor space G . A complete factorial arrangement such that $r_j = r$ for all j is said to consist of r complete replicates.

A factorial arrangement is symmetrical if $k_i = s$ for all $i = 1, 2, \dots, t$, and otherwise it is asymmetrical or mixed. An FA is prime powered if $k_i = p_i^{u_i}$, such that for each i , p_i is a prime and u_i is a natural number greater than or equal to 1. It follows that a factorial arrangement can be symmetrical prime powered or mixed prime powered.

A factorial arrangement is said to be an incomplete factorial arrangement or a fractional factorial design, or more simply, a fractional replicate, if some but not all r_j 's are equal to zero. A fractional replicate is denoted by $\text{FFA}(k_1, k_2, \dots, k_t; m; n; r_1, r_2, \dots, r_N)$ or by FFA if it is clear from the context.

If the levels of the i th factor are made to correspond to the residue classes modulo k_i , i.e., $G_i = \{0, 1, 2, \dots, k_i - 1\}$, then under componentwise addition modulo of the k_i 's, it can be shown that G is an Abelian group. For the symmetrical prime powered s^t factorial each of the G_i 's can be identified with the Galois field $\text{GF}(s)$, where $s = p^u$ and p a prime. It can then be established that G is a t -dimensional vector space over $\text{GF}(s)$. From a geometric viewpoint such a vector space is known as a finite Euclidean geometry $\text{EG}(t, s)$ of dimension t over $\text{GF}(s)$.

Before proceeding further we present an example to illustrate the concepts defined so far.

Example: An industrial experiment was planned to study the effect of both curing time and composition on the tensile strength of plastic compounds.

Three times, 1 hour, 2 hours and 4 hours were selected and four mixes, A, B, C and D were prepared. Observations were to be made on combinations of curing times and compositions. This is a 3×4 factorial with the quantitative factor F_1 = Curing time, the qualitative factor F_2 = Composition, $G_1 = \{1 \text{ hour}, 2 \text{ hours}, 4 \text{ hours}\} = \{1, 2, 4\}$, and $G_2 = \{A, B, C, D\}$. The set of treatment combinations is $G = \{(1, A), (1, B), (1, C), (1, D), (2, A), (2, B), (2, C), (2, D), (4, A), (4, B), (4, C), (4, D)\}$. Note that in using $G_1 = \{1, 2, 4\}$ we have deleted units. Indeed, frequently we use labels to indicate the levels of factors. For our example it is common to use the following sets of labels: $G_1^* = \{0, 1, 2\}$ and $G_2^* = \{0, 1, 2, 3\}$. The set of treatment combinations is then depicted as $G^* = \{(0, 0), (0, 1), (0, 2), (0, 3), (1, 0), (1, 1), (1, 2), (1, 3), (2, 0), (2, 1), (2, 2), (2, 3)\}$ with each element having the obvious real meaning, e.g., $(2, 0) = (4 \text{ hours}, A)$. Since $k_1 = 3$ and $k_2 = 4 = 2^2$, all factorial arrangements in this example are mixed prime powered. The factor space G , or its equivalent representation G^* , is a minimal complete factorial arrangement. The following factorial arrangement in terms of G^* is complete but not minimal: $FA(3, 4; 12; 15; 2, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1) = \{(0, 0), (0, 0), (0, 1), (0, 1), (0, 1), (0, 2), (0, 3), (1, 0), (1, 1), (1, 2), (1, 3), (2, 0), (2, 1), (2, 2), (2, 3)\}$. An example of a fractional replicate in terms of G^* is $FA(3, 4; 5; 6; 1, 1, 0, 0, 0, 0, 0, 1, 1, 2, 0, 0) = \{(0, 0), (0, 1), (1, 3), (2, 0), (2, 1), (2, 1)\}$. Finally note that G^* under componentwise addition modulo 3 and modulo 4 is an Abelian group of order 12.

The Linear Model and Estimation of Effects for a Fractional Factorial Experiment

In this section the linear model for analyzing data from an experiment using a fractional factorial design is introduced. The approach adopted here can be found in several places in the literature (e.g., Raktoc, Hedayat and Federer [1973]) and it conforms to the usual linear model notation found in Graybill [1976] and Searle [1971].

Let D be a factorial arrangement. With each treatment g in D we associate a random variable Y_g , which is called an observation or response. We will assume the univariate case, i.e., Y_g will be one-dimensional and assume values in a one-dimensional Euclidean set. Let Y_D be the $n \times 1$ vector of observations for the factorial arrangement D , where the components of Y_D are the Y_g 's.

In most settings a linear model is associated with minimal complete factorial arrangement D^* in the following way:

$$(i) \quad E[Y_D^*] = X_D^* \beta$$

and

(1)

$$(ii) \quad \text{Cov}[Y_D^*] = \sigma^2 I_N, \quad ,$$

where X_D^* is a known $N \times N$ design matrix, I_N is the identity matrix of order N , and p is the vector of N parameters consisting of $N-1$ factorial effects and the mean. If $X_D^* = X_1 \otimes X_2 \otimes \dots \otimes X_t$, where each X_i is a $k_i \times k_i$ orthogonal matrix with each entry in the first column equal to $1/\sqrt{k_i}$, and \otimes denotes Kronecker product, then β is a vector of factorial effects under the product definition. This approach is especially applicable under the orthogonal polynomial and Helmert polynomial settings. For the symmetrical prime powered factorial the entries of X_D^* can be obtained from a fixed basic orthogonal matrix by using the geometric definition of effects. The model for any fractional factorial design D is induced by (1) in the sense that the design matrix X_D is read off from X_D^* , taking repetitions of treatment combinations into account.

The most practical partitioning of the parametric vector is $\beta' = (\beta_1' : \beta_2' : \beta_3')$, where β_1 is an $N_1 \times 1$ vector to be estimated, β_2 is an $N_2 \times 1$ vector not of interest and not assumed to be known, and β_3 is an $N_3 \times 1$ vector of parameters

assumed to be known (which without loss of generality can be taken to be zero), such that $1 \leq N_1 \leq N$, $0 \leq N_2 \leq N-1$ and $0 \leq N_3 = N - N_1 - N_2 \leq N-1$. This partitioning explicitly leads to the following four cases:

$$\begin{aligned} (i) \quad N_1 = N, N_2 = N_3 = 0, & \quad (ii) \quad N_2 = 0, N_3 \neq 0, \\ (iii) \quad N_2 = 0, N_3 \neq 0 \quad \text{and} & \quad (iv) \quad N_2 \neq 0, N_3 = 0. \end{aligned} \quad (2)$$

Case (i) may be viewed as a special case of (ii) by letting β_1 exhaust β so that $N_3 = 0$. Similarly, case (iv) can be considered a special case of (iii) by letting β_1 and β_2 exhaust β so that $N_3 = 0$. It thus suffices to analyze cases (ii) and (iii) in (2) above.

Denote a parameter in β by the symbol $\beta_1^{x_1} \beta_2^{x_2} \dots \beta_t^{x_t}$, where (x_1, x_2, \dots, x_t) is an element of $G = \prod_{i=1}^t G_i$, $G_i = \{0, 1, 2, \dots, k_i - 1\}$. Then $\beta_1^0 \beta_2^0 \dots \beta_t^0$ is called the mean, and a factorial effect $\beta_1^{u_1} \beta_2^{u_2} \dots \beta_t^{u_t}$ is said to be of order k if exactly k of the exponents are non-zero. A fractional factorial design D is said to be of resolution R if all factorial effects up to order k are estimable, where k is the greatest integer less than $R/2$, under the assumption that all factorial effects of order $R-k$ and higher are zero. When $R=2r$, then the design is known as a design of even resolution, and for $R=2r+1$ the design is said to be of odd resolution. Thus resolution 3 designs allow estimation of all main effects (i.e., effects of order 1) under the assumption that all interactions (i.e., effects of order 2 or higher) are zero. Designs of resolution 4 allow estimation of all main effects under the assumption that interactions of order 3 or higher (i.e., effects of order greater than or equal to 3) are zero without assuming that two-factor interactions (i.e., effects of order 2) are equal to zero. Note that designs of odd resolution belong to case (ii) and designs of even resolution belong to case (iii), respectively, of (2) above.

The model for any fractional factorial design D under case (ii) is given by:

$$E[Y_D] = X_{D1}\beta_1 \quad \text{and} \quad \text{Cov}[Y_D] = \sigma^2 I_n, \quad (3)$$

where the design matrix X_{D1} is simply read off from X_D^* of (1), taking repetitions of treatment combinations into account. Similarly, the design matrix $[X_{D1}:X_{D2}]$ for a design D under case (iii) is obtained from X_D^* as:

$$E[Y_D] = [X_{D1}:X_{D2}][\beta_1':\beta_2']' \quad \text{and} \quad \text{Cov}[Y_D] = \sigma^2 I_n. \quad (4)$$

The best linear unbiased estimator (BLUE) of β_1 and the covariance for the two cases are given, respectively, by (5) and (6) below:

$$\hat{\beta}_1 = [X_{D1}'X_{D1}]^{-1}X_{D1}'Y_D \quad \text{and} \quad \text{Cov}[\hat{\beta}_1] = [X_{D1}'X_{D1}]^{-1}\sigma^2, \quad (5)$$

$$\hat{\beta}_1 = [X_{D1}'X_{D1} - X_{D1}'X_{D2}(X_{D2}'X_{D2})^{-1}X_{D2}'X_{D1}]^{-1}[X_{D1}' - X_{D1}'X_{D2}(X_{D2}'X_{D2})^{-1}X_{D2}']Y_D$$

(6)

and

$$\text{Cov}[\hat{\beta}_1] = [X_{D1}'X_{D1} - X_{D1}'X_{D2}(X_{D2}'X_{D2})^{-1}X_{D2}'X_{D1}]^{-1}\sigma^2.$$

In expression (6) A^- denotes a generalized inverse of A. For brevity the covariances in either case will be written as $M_D^{-1}\sigma^2$, where M_D^{-1} is known as the covariance matrix and M_D itself is called the information matrix. An unbiased estimator of σ^2 is obtained by utilizing the BLUE's in (5) and (6), viz., $\hat{\sigma}^2 = (Y_D - X_{D1}\hat{\beta}_1)'(Y_D - X_{D1}\hat{\beta}_1)/(n - N_1)$ for case (ii), and for case (iii), $\hat{\sigma}^2 = (Y_D - X_{D1}\hat{\beta}_1 - X_{D2}\tilde{\beta}_2)'(Y_D - X_{D1}\hat{\beta}_1 - X_{D2}\tilde{\beta}_2)/(n - N_1)$, where $\tilde{\beta}_2 = (X_{D2}'X_{D2})^{-1}[X_{D2}'Y_D - X_{D2}'X_{D1}\hat{\beta}_1]$. Under the assumption of normality, tests of hypotheses and confidence interval estimators for the vector β_1 can be obtained as indicated, for example, in Graybill [1976].

Optimal Fractional Factorial Experiments

The problem of choosing an optimal fractional factorial design is discussed in this section using optimality criteria developed by Kiefer [1959] and Hedayat, Raktue and Federer [1974].

Let \underline{D} be a class of competing fractional factorial designs in either setting (ii) or (iii) of the partitioning in (2) of the previous section. Assume that each design $D \in \underline{D}$ is capable of providing an unbiased estimator for β_1 . There are several optimality criteria based on the covariance matrix M_D^{-1} of the BLUE of β_1 . The most popular ones are based on the spectrum or set of characteristic roots of M_D^{-1} . Denoting the roots of M_D^{-1} in increasing order of magnitude by $\lambda_1, \lambda_2, \dots, \lambda_{N_1}$ we have the following functionals:

$$(a) \quad \pi\lambda_i = |M_D^{-1}|, \quad (b) \quad \Sigma\lambda_i = \text{Trace } M_D^{-1}$$

(7)

and

$$(c) \quad \lambda_{N_1} = \max(\lambda_1, \lambda_2, \dots, \lambda_{N_1})$$

A design which minimizes over \underline{D} the criteria in (a), (b) and (c), respectively, is known as a d-optimal design, a-optimal design and e-optimal design. Statistical interpretations of these criteria are available and they may be found in Kiefer [1959]. It should be noted that one may base these optimality criteria on the spectrum of the information matrix M_D rather than on that of M_D^{-1} .

Another criterion, which does not rely on the covariance matrix M_D^{-1} , was developed by Hedayat, Raktue and Federer [1974]. If in the settings (ii) and (iii) of (2) in the previous section the assumption that $\beta_3 = 0$ is in doubt, then $E[\hat{\beta}_1] = \beta_1 + A_D \beta_3$, where A_D is known as the alias matrix of the design D relative to β_1 and β_3 (e.g., for case (iii) of (2) $A_D = (X'_{D1} X_{D1})^{-1} X'_{D1} X_{D2}$). The norm $\|A_D\| = [\text{Trace}(A'_D A_D)]^{\frac{1}{2}}$ was proposed by Hedayat et al. [1974] for the

selection of an optimal design and a design is said to be alias optimal if it minimizes $\|A_D\|$ over D .

Apart from these criteria one may impose other desirable properties on D for the selection of a design, such as orthogonality (i.e., M_D^{-1} is diagonal) or balancedness (i.e., $M_D^{-1} = aI + bJ$, where J is a square matrix of order N_1 all whose elements are 1's). Orthogonality implies uncorrelatedness of the estimators of the elements of β_1 and balancedness implies equal variances and equal covariances of the estimators. These concepts have been generalized to partial orthogonality and partial balancedness (e.g., see Srivastava and Anderson [1970]).

If the mean is the first element in β_1 , then the first element of the vector $\beta_1 + A_D \beta_3$ is known as the generalized defining relationship of D relative to β_1 and β_3 and the whole vector itself is called the aliasing structure of D relative to β_1 and β_3 . The aliasing structure for a symmetrical prime powered fractional factorial design becomes tractable via group-theoretic techniques if the design is regular; i.e., it is a subspace (or coset of a subspace) when the complete set of treatment combinations is viewed as the t -dimensional vector space over the Galois field $GF(s)$ (e.g., see Raktoe, Pesotan and Federer [1979]). For the 2^t factorial the generalized defining relationship is known as the defining contrast (e.g., see Cochran and Cox [1957]).

Construction of Fractional Factorial Designs

The construction of an optimal design in either setting (ii) or (iii) of (2) is by no means a simple matter since it involves the design parameters $k_1, k_2, \dots, k_t, m, n, r_1, r_2, \dots, r_N, N_1, N_2, N_3$ and selection of the optimality criterion. Indeed, there is a formidable combinatorial problem associated with finding for the $k_1 \times k_2 \times \dots \times k_t$ factorial all designs which

simply lead to unbiased estimation of β_1 in (ii) or (iii) of (2), let alone obtaining the optimal ones. There is no unique method available for all factorials and depending on the nature of the factorial one may utilize various techniques to obtain useful designs.

Raktoe, Hedayat and Federer [1973] list twenty-four methods in their unpublished monograph. These are:

- (1) Trial and error and/or computer methods;
- (2) Hadamard matrix methods;
- (3) Confounding techniques;
- (4) Group theory methods;
- (5) Finite geometrical methods;
- (6) Algebraic decomposition techniques;
- (7) Combinatorial-topological methods;
- (8) Fold-over techniques;
- (9) Collapsing of levels methods;
- (10) Composition (direct product and direct sum) methods;
- (11) Permutation of levels and/or factors methods.
- (12) Coding theory methods;
- (13) Orthogonal array techniques;
- (14) Partially balanced array techniques;
- (15) Orthogonal Latin square methods;
- (16) Block design techniques;
- (17) Weighing design techniques;
- (18) F-Square techniques;
- (19) Lattice design methods;
- (20) Graph-theoretical methods;
- (21) One-at-a-time methods;

- (22) Inspection methods;
- (23) Patterned matrix methods; and
- (24) Cutting and adjoining matrix methods.

In order to demonstrate the complexity of the problems, an illustration is given of the general combinatorial problem for case (ii) of (2) for resolution 3 designs in their simplest possible setting. Assume that the mean is also of interest of estimation so that a minimal (or saturated) resolution 3 design calls for $N_1 = m = n = \sum k_i - t + 1$ distinct treatment combinations for estimation of β_1 since there are $N_1 = \sum (k_i - 1) + 1$ parameters in β_1 . We have seen that a necessary and sufficient condition for estimating β_1 is that the rank of X_{D1} (or of $X'_{D1} X_{D1}$) is equal to m . Denote the class of possible designs by \underline{D}_m ; then clearly its cardinality is equal to:

$|\underline{D}_m| = C_m^N = (N!)/(m!)(N-m)!$. Denote by $\underline{D}_{m,m}$ the class of designs in \underline{D}_m which allow estimation of β_1 and by $\underline{D}_{m,0}$ the singular (viz., $|X_{D1}| = 0$) class of designs. The cardinality of $\underline{D}_{m,0}$ (and hence that of $\underline{D}_{m,m}$) is not known in general at present. For the 2^t factorial it has been enumerated for $t \leq 7$, which can be found in Raktoe [1979]:

	t					
	2	3	4	5	6	7
$ \underline{D}_m = C_{t+1}^{2^t}$	4	70	4368	906192	621216192	1429702652400
$ \underline{D}_{m,0} $	0	12	1360	350000	255036992	571462430224
$ \underline{D}_{m,m} $	4	58	3008	556192	366179200	858240222176
$ \underline{D}_{m,0} / C_{t+1}^{2^t}$	0	.1714	.3114	.3862	.4105	.3997
$ \underline{D}_{m,m} / C_{t+1}^{2^t}$	1	.8286	.6886	.6138	.5895	.6003

It may be shown that the proportion of singular designs goes to zero as t

goes to infinity for the 2^t factorial.

Using Helmert polynomials and corresponding non-normalized column-wise orthogonal matrices in (1) for the $k_1 \times k_2 \times \dots \times k_t$ factorial, one may deduce under the determinant criterion that for a saturated resolution III design $D \in D_{-m}$:

$$\prod_{i=1}^t (k_i!)^2 \leq |\det X'_{D1} X_{D1}| \leq \prod_{i=1}^t (k_i!)^2 m^t \prod_{i=1}^t k_i^{-k_i} \quad (8)$$

The lower bound in (7) is attained by the one-at-a-time design

$D^* = \{(000\dots 0), (100\dots 0), (200\dots 0), \dots, (k_1 - 100\dots 0), \dots, (010\dots 0), (020\dots 0), \dots, (0k_2 - 10\dots 0), \dots, (000\dots 01), (000\dots 02), \dots, (000\dots 0k_t - 1)\}$, which is a

least d-optimal resolution 3 design. The upper bound is attained if and only if an orthogonal design can be constructed. For the 2^t factorial the bound is achieved whenever a Hadamard matrix of order $t+1$ exists. A necessary condition for this is that $t+1 \equiv 0 \pmod{4}$. Hadamard matrices have been constructed for all $t+1 \leq 200$ so that minimal d-optimal resolution 3 designs are available for all 2^t factorials, where $t = 4s - 1$ and $s = 1, 2, \dots, 50$. For $t+1 \not\equiv 0 \pmod{4}$ other techniques have been used apart from computer methods. Examples of minimal d-optimal resolution III designs for the 2^t factorial are:

t	d-optimal design
2	$\{(00), (10), (01)\}$
3	$\{(000), (110), (101), (011)\}$
4	$\{(0000), (1110), (1101), (1011), (0111)\}$
5	$\{(00000), (11100), (11010), (11001), (10111), (01111)\}$
6	$\{(000000), (111000), (110110), (110101), (101100), (101011), (011111)\}$
7	$\{(0000000), (111000), (1100110), (1010101), (1001011), (0110011), (0101101), (0011110)\}$

These designs are such that the spectrum of the information matrix is invariant under the group of level permutations.

Some of the references listed below deal with constructions of other types of fractional factorial designs, such as resolution 4 and 5 designs which are not necessarily minimal.

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